Inversion of R_{rs} to IOPs: where we are & where we (might) want to go

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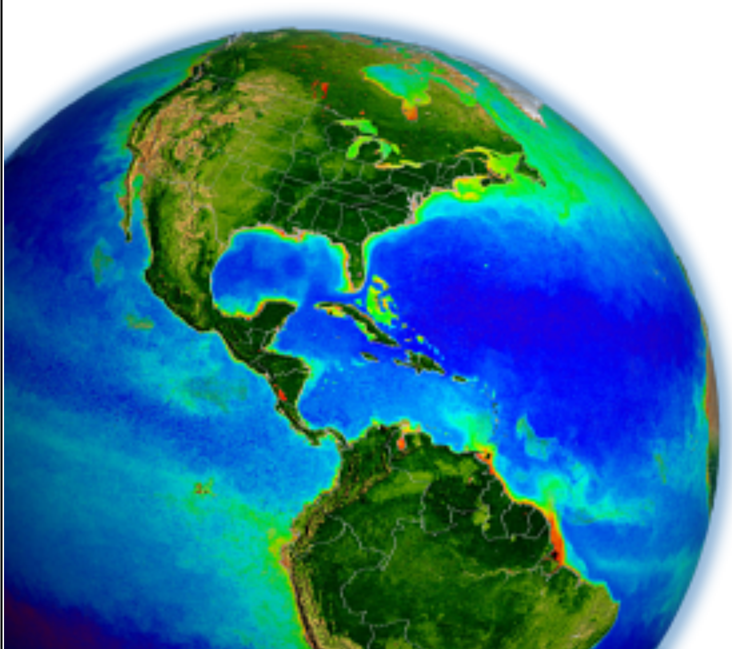
NASA Goddard Space Flight Center

PACE Science Team Meeting

14-16 Jan 2015



purpose of this presentation

(1) provide an opportunity for IOP aficionados to have a frank, collaborative discussion on the state-of-the-art in IOP determinations, our forthcoming challenges, & where we want to be in the next two years

(2) provide the above in such a manner to effectively convey the state-of-the-art, plus our ideas & concerns, to the non-aficionados

for the non-aficionados in the room

what are marine inherent optical properties (IOPs)?

spectral absorption & volume scattering coefficients

- total absorption (a) & its subcomponents (a_w, a_p, a_{ph}, a_d, a_g)
- volume scattering function ($\beta(\theta)$; VSF) & total scattering (b)
- total backscattering (b_b) & its subcomponents (b_{bw}, b_{bp})
- beam attenuation of particles (c_p)

what can marine IOPs tell me?

they describe the contents of the upper ocean

- phytoplankton abundance & community structure
- particle size distributions
- non-algal suspended particle abundance
- particulate & dissolved carbon abundance
- diffuse attenuation / water clarity

PACE SDT recommend measurement ranges for an OCI

baseline ("desired"): 1% & 99% positions of frequency distribution
threshold ("required"): 5% & 95% positions of frequency distribution

a	0.02	0.03	0.7	1.8	m^{-1}
a_{ph}	0.003	0.007	0.7	1.2	m^{-1}
a_d	0.0004	0.001	0.3	0.6	m^{-1}
a_g	0.002	0.003	0.5	0.9	m^{-1}
b_{bp}	0.0003	0.001	0.003	0.1	m^{-1}
c	0.03	0.1	0.5	10	m^{-1}

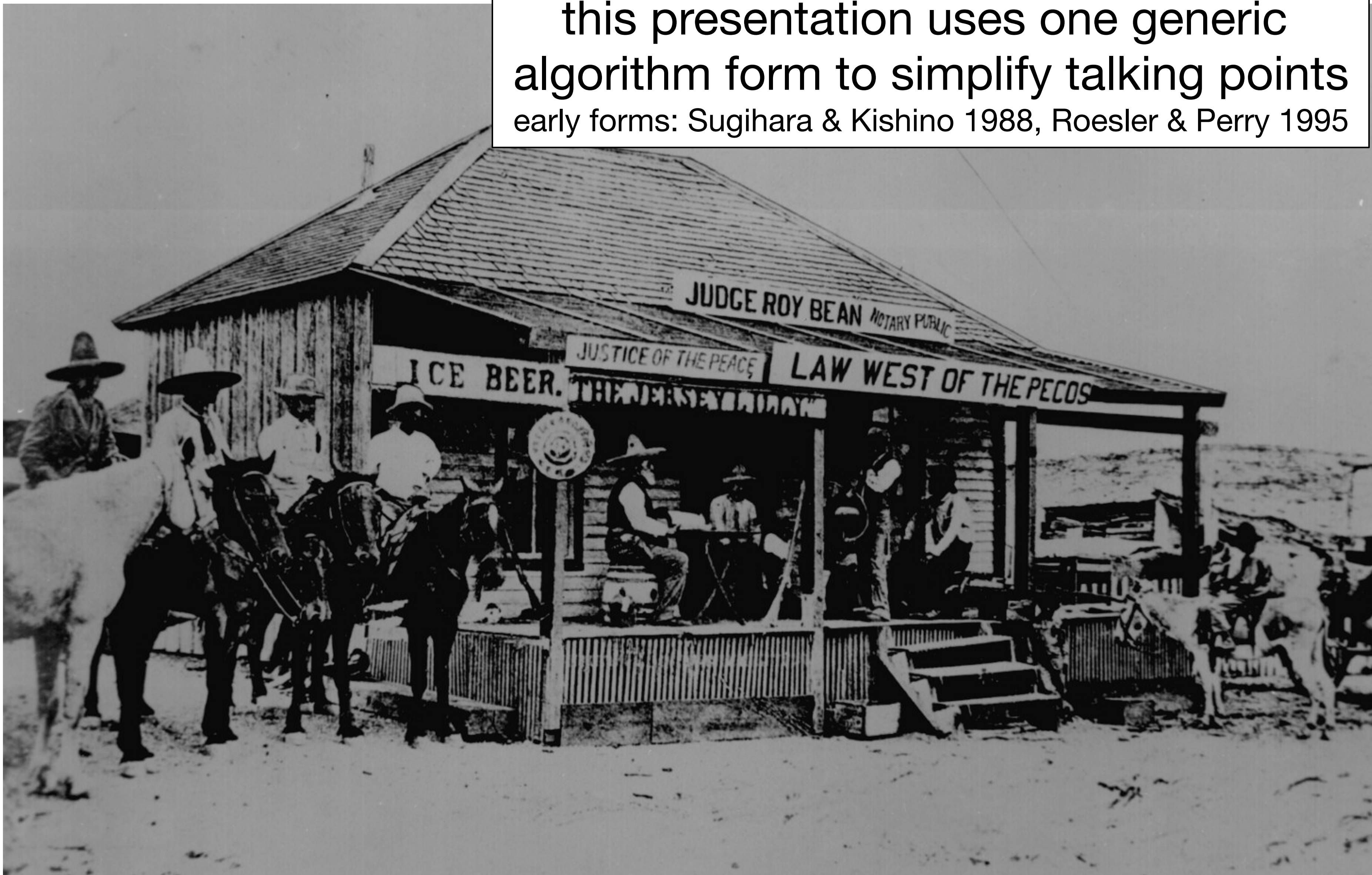
Values for 443 nm. Ranges estimated using multiple in situ data sets. From PACE SDT table A-1 (also from previous ACE ST white paper).

No (obvious) satellite IOP accuracy/precision requirements (yet).

instruments & algorithms – many exist

this presentation uses one generic algorithm form to simplify talking points

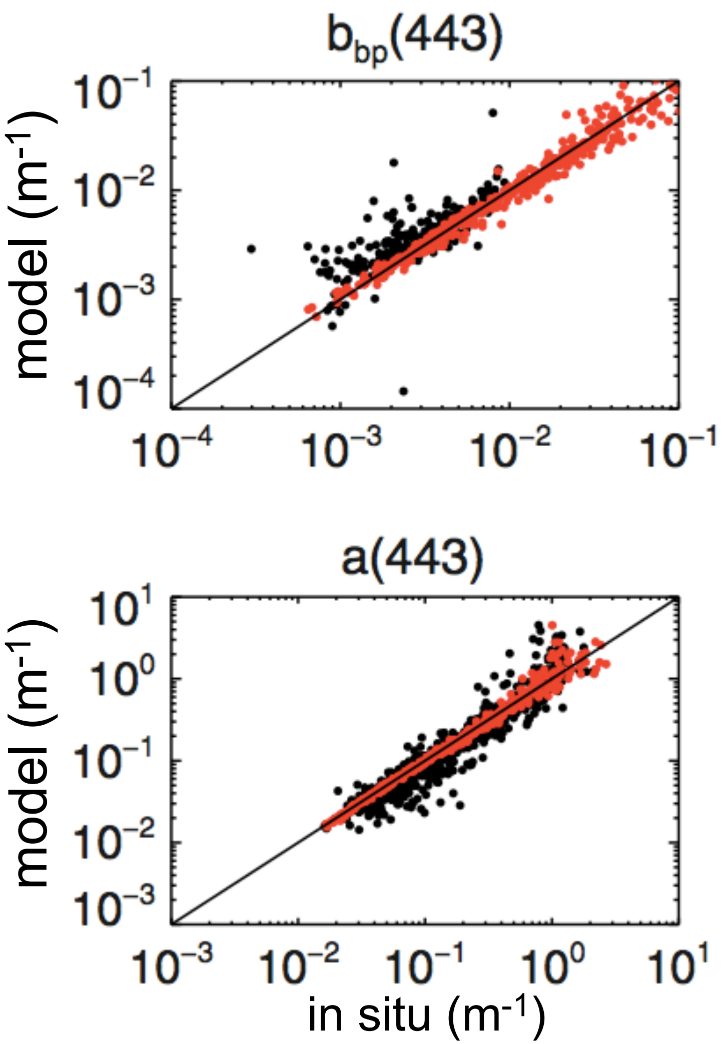
early forms: Sugihara & Kishino 1988, Roesler & Perry 1995



where are we today?

most algorithm reasonably retrieve total IOPs over a large dynamic range

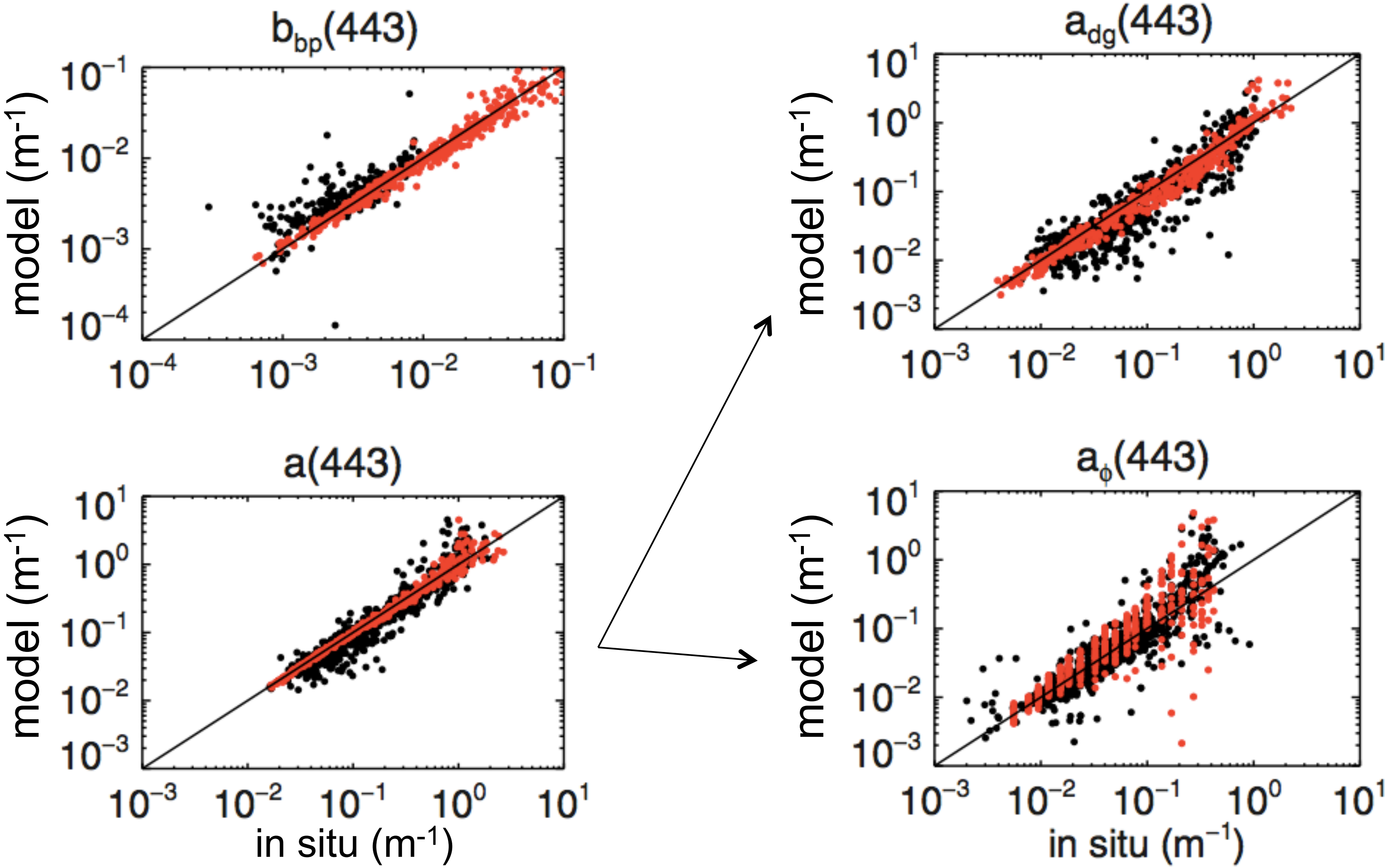
color key: in situ data, synthesized data



where are we today?

dividing totals into subcomponents adds variability & uncertainty

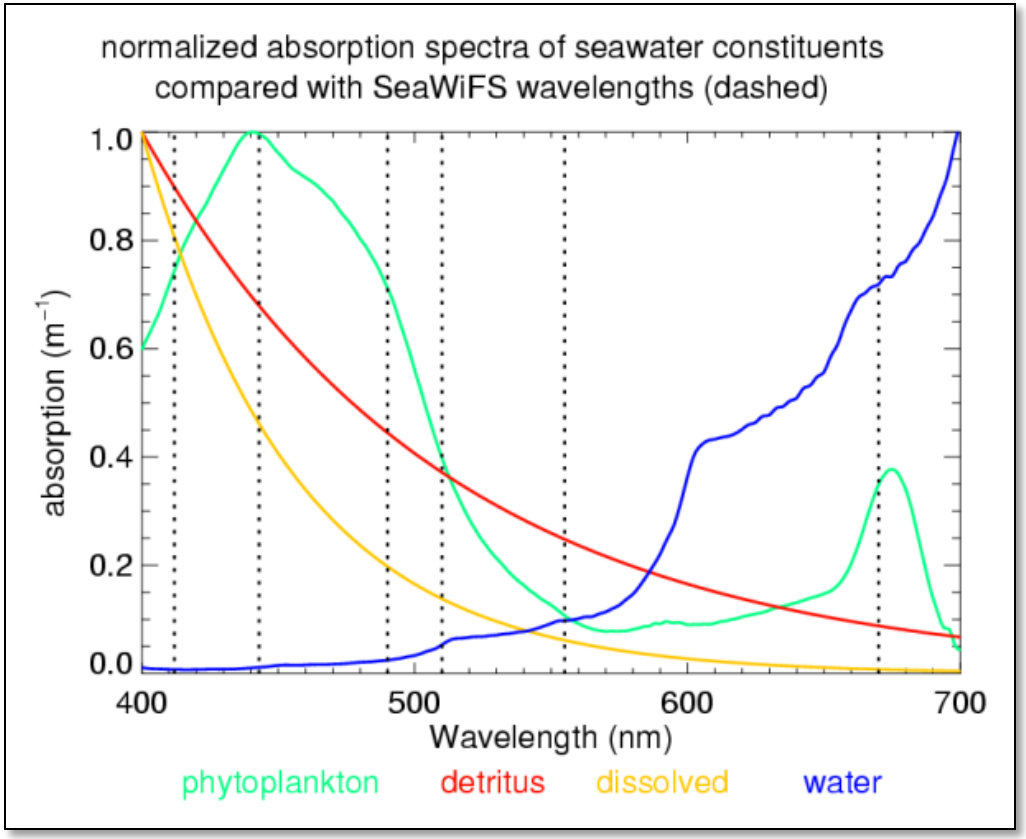
color key: in situ data, synthesized data

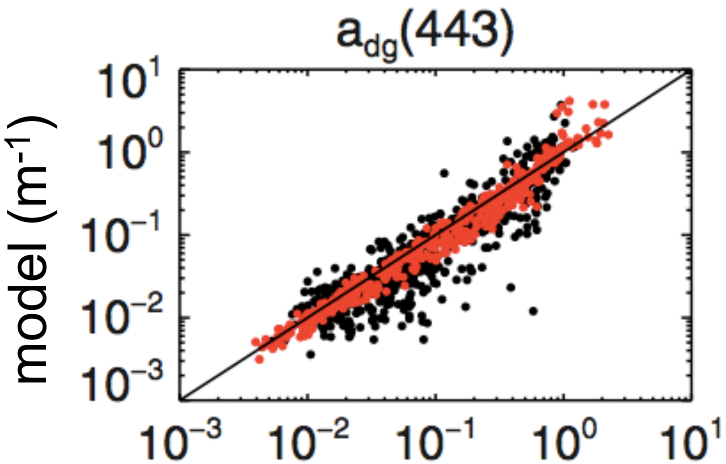


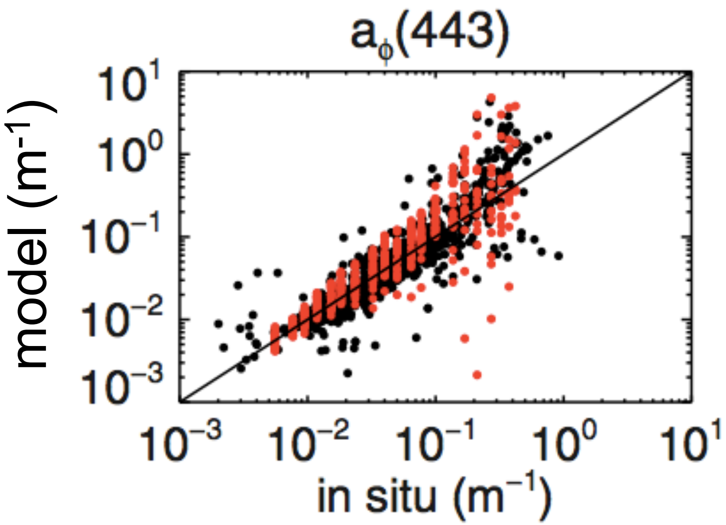
where are we today?

idea is that subcomponents differ optically at satellite wavelengths

but individual subcomponents vary spatially / temporally / biogeochemically / physiologically







where are we today?

many comprehensive analyses of algorithms & instruments exist

Reports of the International Ocean-Colour Coordinating Group

An Affiliated Program of the Scientific Committee on Oceanic Research (SCOR)
An Associate Member of the Committee on Earth Observation Satellites (CEOS)

IOCCG Report Number 5, 2006

Remote Sensing of Inherent Optical Properties: Fundamentals, Tests of Algorithms, and Applications

Editor:
ZhongPing Lee (Naval Research Laboratory, Stennis Space Center, USA)

Report of an IOCCG working group on ocean-colour algorithms, chaired by ZhongPing Lee and based on contributions from (in alphabetical order):

Robert Arnone, Marcel Babin, Andrew H. Barnard, Emmanuel Boss, Jennifer P. Cannizzaro, Kendall L. Carder, F. Robert Chen, Emmanuel Devred, Roland Doerffer, KePing Du, Frank Hoge, Oleg V. Kopelevich, ZhongPing Lee, Hubert Loisel, Paul E. Lyon, Stéphane Maritorena, Trevor Platt, Antoine Poteau, Collin Roesler, Shubha Sathyendranath, Helmut Schiller, Dave Siegel, Akihiko Tanaka, J. Ronald V. Zaneveld

Series Editor: Venetia Stuart

first comprehensive survey & evaluation of algorithms

Generalized ocean color inversion model for retrieving marine inherent optical properties

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Ocean color measured from satellites provides daily, global estimates of marine inherent optical properties (IOPs). Semi-analytical algorithms (SAAs) provide one mechanism for inverting the color of the water observed by the satellite into IOPs. While numerous SAAs exist, most are similarly constructed and few are appropriately parameterized for all water masses for all seasons. To initiate community-wide discussion of these limitations, NASA organized two workshops that deconstructed SAAs to identify similarities and uniqueness and to progress toward consensus on a unified SAA. This effort resulted in the development of the generalized IOP (GIOP) model software that allows for the construction of different SAAs at runtime by selection from an assortment of model parameterizations. As such, GIOP permits isolation and evaluation of specific modeling assumptions, construction of SAAs, development of regionally tuned SAAs, and execution of ensemble inversion modeling. Working groups associated with the

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first comprehensive evaluation of algorithm similarities/differences

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modern survey & evaluation of algorithms

The Ocean Colour Climate Change Initiative: III. A round-robin comparison on in-water bio-optical algorithms

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ABSTRACT

Satellite-derived remote-sensing reflectance can be used for mapping biogeochemically relevant variables, such as the chlorophyll concentration and the Inherent Optical Properties (IOPs) of the water, at global scales for use in climate-change studies. Prior to generating such products, suitable algorithms have to be selected that are appropriate for the purpose. Algorithm selection needs to account for both qualitative and quantitative requirements. In this paper we develop an objective methodology designed to rank the quantitative performance of a suite of bio-optical models. The objective classification is applied using the NASA bio-Optical Marine Algorithm Dataset (NOMAD). Using in situ R_{rs} as input to the models, the performance of eleven semi-analytical models, as well as five empirical chlorophyll algorithms and an empirical diffuse attenuation coefficient algorithm, is ranked for spectrally-resolved IOPs, chlorophyll concentration and the diffuse attenuation coefficient at 489 nm. The sensitivity of the objective classification and the uncertainty in the ranking are tested using a Monte-Carlo approach (bootstrapping). Results indicate that the performance of the semi-analytical models varies depending on the product and wavelength of interest. For chlorophyll retrieval, empirical algorithms perform better than semi-analytical models, in general. The performance of these empirical models reflects either their immunity to scale errors or instrument noise in R_{rs} data, or simply that the data used for model parameterisation were not independent of NOMAD. Nonetheless, uncertainty in the classification suggests that the performance of some semi-analytical algorithms at retrieving chlorophyll is comparable with the empirical algorithms. For phytoplankton absorption at 443 nm, some semi-analytical models also perform with similar accuracy to an empirical model. We discuss the potential biases, limitations and uncertainty in the approach, as well as additional qualitative considerations for algorithm selection for climate-change studies. Our classification has the potential to be routinely implemented, such that the performance of emerging algorithms can be compared with existing algorithms as they become available. In the long-term, such an approach will further aid algorithm development for ocean-colour studies.

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where are we today?

in general, not all IOPs retrieved by contemporary approaches

passive ocean color instruments do not measure forward scattering

a_{dg}

- total absorption (a) & its subcomponents (a_w, a_p, a_{ph}, a_d, a_g)
- volume scattering function ($\beta(\theta)$; VSF) & total scattering (b)
- total backscattering (b_b) & its subcomponents (b_{bw}, b_{bp})
- beam attenuation of particles (c_p)

limited by data availability, instruments, & environmental variability

one size does not fit all & we cannot yet measure everything everywhere

- comprehensive data sets limited in space & time
- synthesized data sets cannot represent all conditions
- instrument protocols to be updated / revised
- in situ instrumentation to be improved / enhanced
- biogeochemical / physiological relationships to be improved

what IOP improvements do we expect out of PACE?

for this presentation, assume improved A/C & therefore excellent R_{rs} (and historical secondary data products)

hyperspectral – ability to observe pigments other than chlorophyll & their absorption (backscattering?) features
- phytoplankton abundance & community composition

UV – ability to better separate CDOM (dissolved organic material) from chlorophyll; potential to separate CDOM & non-algal particles
- carbon stocks & fates
- water clarity, offshore tracers, resuspension events

polarimetry – depolarization ratio -> backscattering ratio -> beam attenuation spectrum, bulk composition of organics vs. inorganics, & better size information; volume scattering functions?
- particle sizes & composition
- volume scattering / R_{rs}-IOP relationships

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polarimetry – enable estimation of backscattering ratios, leading to beam attenuation spectra, bulk composition of organics vs. inorganics, & better size information; measure volume scattering?
- particle sizes & composition
- volume scattering / R_{rs}-IOP relationships

bird's-eye view of challenges

algorithms:

many algorithms; all with strengths & weaknesses; best combo not identified
making assumptions regarding component spectral shapes
assigning & propagating **uncertainties**

data:

paucity of complete datasets – full suites of R_{rs} plus IOPs (plus stocks?)
existing synthesized data highly useful, but cannot represent all conditions
how to improve use of other **environmental information** to better constrain biogeochemical / physiological assumptions in spectral shapes?

instrumentation / methods:

expanding the spectral domain (e.g., into the UV)
multi- versus hyperspectral instrumentation (e.g., backscattering)
uncertainties, revised measurement protocols, NIST-traceable standards

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outline of forthcoming discussion

remainder of presentation will provide a general review of challenges associated with algorithms

the floor will be open for algorithm-related comments

the floor will be open for discussion challenges associated with data, uncertainties, environmental variability, measurement methods, & other related topics of interest

absorbing & scattering components are additive & can be expressed as the product of their shape & magnitude

$$a(\lambda) = a_w(\lambda) + a_{dg}(\lambda) + a_\phi(\lambda)$$

$$a(\lambda) = a_w(\lambda) + \underbrace{M_{dg}}_{\substack{\text{eigenvalue}\\ \text{(magnitude)}}} \underbrace{a^*_{dg}(\lambda)}_{\substack{\text{eigenvector}\\ \text{(shape)}}} + M_\phi a^*_\phi(\lambda)$$

$$b_b(\lambda) = b_{bw}(\lambda) + b_{bp}(\lambda)$$

$$b_b(\lambda) = b_{bw}(\lambda) + M_{bp} b^*_{bp}(\lambda)$$

relating R_{rs} (the satellite) to IOPs (what we want)

$$R_{rs}(\lambda) = G(\lambda)\frac{b_{bw}(\lambda) + M_{bp}b^{*}_{bp}(\lambda)}{b_{bw}(\lambda) + M_{bp}b^{*}_{bp}(\lambda) + a_{w}(\lambda) + M_{dg}a^{*}_{dg}(\lambda) + M_{ph}a^{*}_{ph}(\lambda)}$$

relating R_{rs} (the satellite) to IOPs (what we want)

$$R_{rs}(\lambda) = \overline{G(\lambda)} \frac{\overline{b_{bw}(\lambda)} + \overline{M_{bp}}\,\overline{b_{bp}^{*}(\lambda)}}{\underline{b_{bw}(\lambda)} + \underline{M_{bp}}\,\underline{b_{bp}^{*}(\lambda)} + \underline{a_w(\lambda)} + \underline{M_{dg}}\,\underline{a_{dg}^{*}(\lambda)} + \underline{M_{ph}}\,\underline{a_{ph}^{*}(\lambda)}}$$

terms with **blue bars** have pre-assigned spectral shapes associated with them (known or modeled)

find combination of ***M'***s (**red bars**) such that right hand side best reconstructs left hand side

the R_{rs} to IOP relationship

$$R_{rs}(\lambda) = G(\lambda)\underbrace{\boxed{\frac{b_{bw}(\lambda) + M_{bp}b^{*}_{bp}(\lambda)}{b_{bw}(\lambda) + M_{bp}b^{*}_{bp}(\lambda) + a_{w}(\lambda) + M_{dg}a^{*}_{dg}(\lambda) + M_{ph}a^{*}_{ph}(\lambda)}}}_{=\,u}$$

$$R_{rs}(\lambda) = G_1(\lambda)\, u(\lambda) + G_2(\lambda)\, u(\lambda)^2$$

several parameterizations of *G* exist

- are any valid in the UV?
- is spectral dependence required?
- does the quadratic offer an advantage over the linear ($G_2 = 0$)?

other analytical relationships exist that more explicitly include VSF info

- do these offer improvements?
- use direct VSF measurement (polarimetery?) or regional tuning?

ZP Lee slides to follow

seawater values

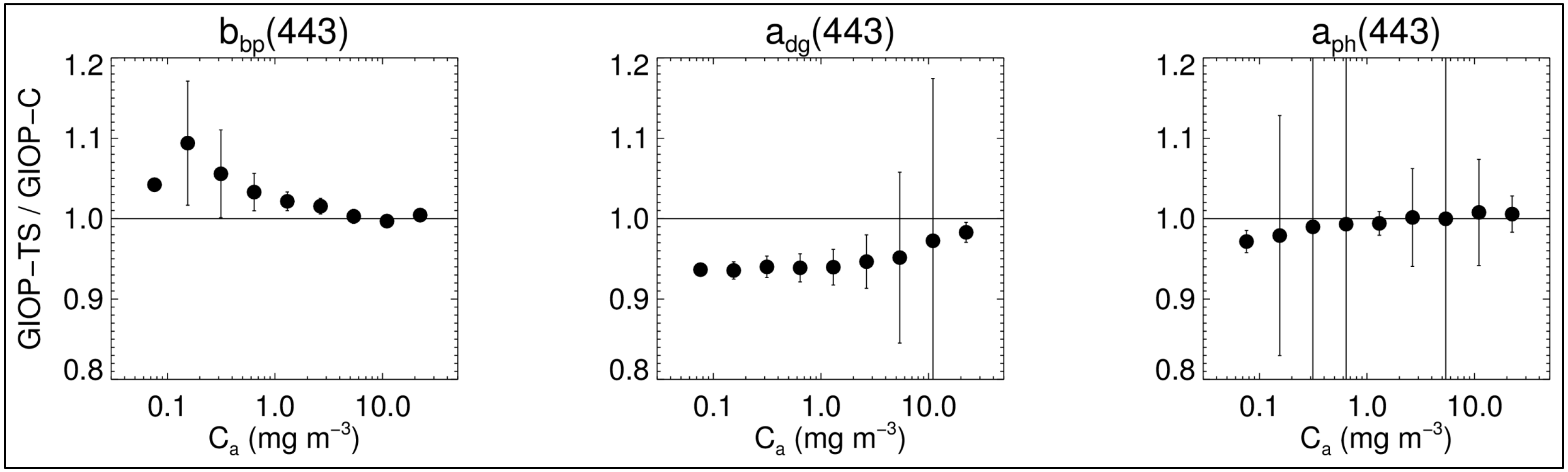
$$R_{rs}(\lambda) = G(\lambda)\frac{b_{bw}(\lambda) + M_{bp}b_{bp}^{*}(\lambda)}{b_{bw}(\lambda) + M_{bp}b_{bp}^{*}(\lambda) + a_{w}(\lambda) + M_{dg}a_{dg}^{*}(\lambda) + M_{ph}a_{ph}^{*}(\lambda)}$$

b_{bw}

- include temperature & salinity dependence
- revise depolarization ratio
- desire improved ancillary sources

a_w

- include temperature & salinity dependence
- revisit values / methods of determination



the inversion method

$$R_{rs}(\lambda) = \overline{G(\lambda)} \frac{\overline{b_{bw}(\lambda)} + \overline{M_{bp}}\,\overline{b^*_{bp}(\lambda)}}{\underline{b_{bw}(\lambda)} + \underline{M_{bp}}\,\underline{b^*_{bp}(\lambda)} + \underline{a_w(\lambda)} + \underline{M_{dg}}\,\underline{a^*_{dg}(\lambda)} + \underline{M_{ph}}\,\underline{a^*_{ph}(\lambda)}}$$

find combination of ***M'***s such that right side best reconstructs left side

many approaches exist, all with strengths & weaknesses

- best-fit, spectral matching to simultaneously solve for *M*
- piecewise spectral decomposition that sequentially solves for *M*
- bulk, band-by-band decomposition
- static and/or dynamic LUTs
- others …

many ways to decompose totals in non-remote sensing literature

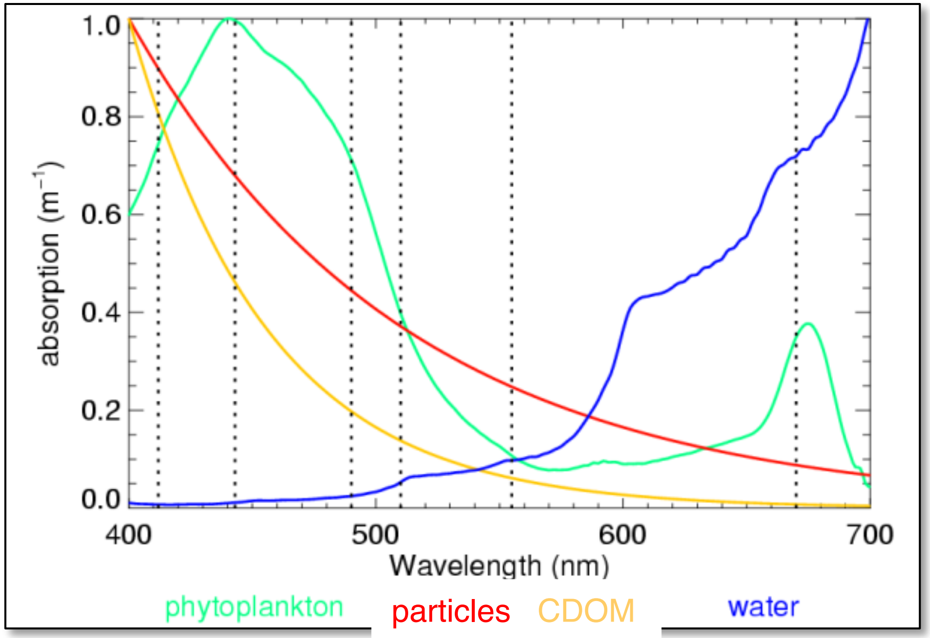
- use most computationally efficient method to solve for totals (a, b_b)
- decompose totals into subcomponents in second step

the R_{rs} to IOP relationship

$$R_{rs}(\lambda) = G(\lambda)\frac{b_{bw}(\lambda) + M_{bp} b^*_{bp}(\lambda)}{b_{bw}(\lambda) + M_{bp} b^*_{bp}(\lambda) + a_w(\lambda) + M_{dg} a^*_{dg}(\lambda) + M_{ph} a^*_{ph}(\lambda)}$$

typical expressions for spectral shapes

- $b^*_{bp}(\lambda) = \lambda^{-\eta}$
- $a^*_{dg}(\lambda) = \exp(-S\,\lambda)$
- $a^*_{ph}(\lambda)$ = tabulated or some function of *Chl* / phytoplankton



generations of semi-analytical algorithms for retrieving IOPs

assigning eigenvectors (spectral shapes) – one size DOES NOT fit all

First Generation: Constant spectral shapes (eigenvectors) assigned to all unknown parameters (eigenvalues).

Roesler and Perry 1995; Hoge and Lyon 1996; Maritorena et al. 2002 (**GSM**)

Second generation: Spectral shapes for unknown parameters calculated dynamically, often using empirical relationships dependent on ratios of Rrs.

Lee et al. 2002 (**QAA**); Smyth et al. 2006 (**PML**); Werdell et al. 2013 (**GIOP-DC**)

Third generation: Ranges of spectral shapes for unknown parameters applied iteratively. Final unknown parameters calculated as median of all valid values retrieved during iteration.

Wang et al. 2005; Brando et al. 2012

Towards the next generation: Merge second and third generations, plus consider other ensemble approaches, such as OWTs (Moore et al. 2009), and expand framework to support optically shallow water (Lee et al. 2001).

the R_{rs} to IOP relationship

$$R_{rs}(\lambda) = G(\lambda)\frac{b_{bw}(\lambda) + M_{bp}b^*_{bp}(\lambda)}{b_{bw}(\lambda) + M_{bp}b^*_{bp}(\lambda) + a_w(\lambda) + M_{dg}a^*_{dg}(\lambda) + M_{ph}a^*_{ph}(\lambda)}$$

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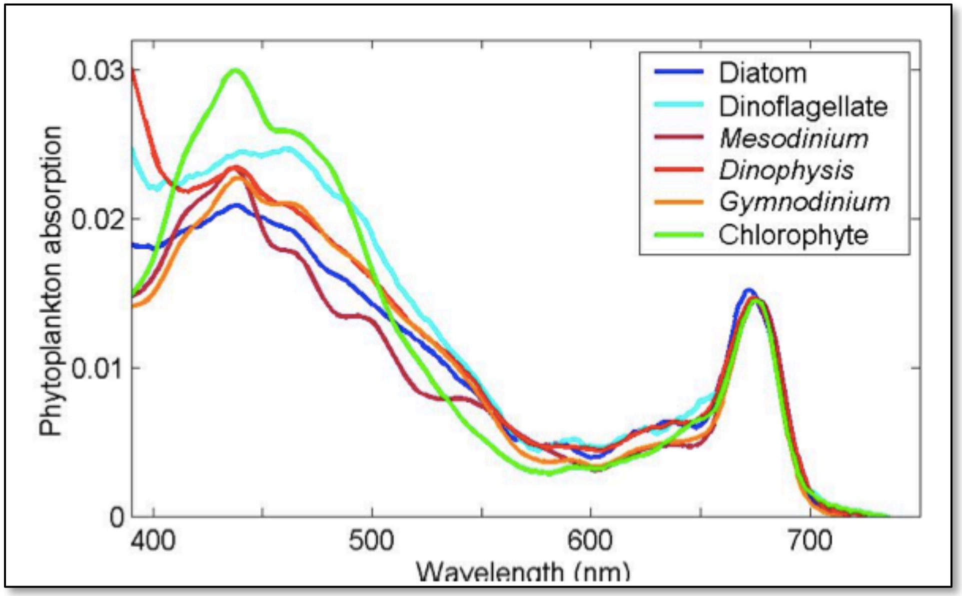

from Roesler et al. 2004

the R_{rs} to IOP relationship

$$R_{rs}(\lambda) = G(\lambda)\frac{b_{bw}(\lambda) + M_{bp}b^*_{bp}(\lambda)}{b_{bw}(\lambda) + M_{bp}b^*_{bp}(\lambda) + a_w(\lambda) + M_{dg}a^*_{dg}(\lambda) + M_{ph}a^*_{ph}(\lambda)}$$

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issues with the parameterization of spectral shapes

- are these expressions valid / the best to use?
- how best to dynamically assign shape parameters pixel-by-pixel?
- expansion into additional subcomponents
- reducing / constraining / avoiding assumptions
- additional free parameters (η, S)?

input uncertainties, cost functions, & output uncertainties

input uncertainties

- need uncertainties on input R_{rs} (match-ups, SNRs, Monte Carlo stats)
- can these uncertainties vary in time & space?
- include uncertainties associated with spectral shapes / in situ data?

cost functions (best-fit spectral matching methods only)

- most (e.g., Levenberg Marquardt) use a χ^2 form
- use of absolute & relative differences?

output uncertainties

- desire pixel-by-pixel uncertainties on output IOP products
- common units of measure of uncertainty?
- a number of methods for calculating / propagating error proposed
- report ranges of feasible solutions?
- what wavelengths?
- quality levels in standard satellite data files?

other topics & challenges

inelastic scattering (Raman, *Chl* / CDOM fluorescence)
- methods to incorporate Raman exist

quality control metrics
- how to define a valid retrieval?
- data ranges / goodness of fit currently used

evaluating improvements
- data values (regression stats, unbiased % differences, RMSD)
- vary by water type or trophic level?
- satellite spatial & temporal coverage
- computational performance
- many products done ok versus single product done exceptionally

incorporating other data products
- polarimetry
- ancillary data (mixed layer depth, temperature, salinity, etc.)

normalizations, bidirectional reflectance functions (BRDF, VSF)

optically shallow water

available tools

satellite (l2gen/SeaDAS) & IDL/Matlab/Python software for evaluating IOP parameterizations / modules (GIOP framework)

data sets (IOP subgroup, synergy with A/C group, proposed work by Mitchell & Lee & data from other proposals)

what else?

tangible GSFC contributions to the ST

implementation / evaluation of Raman corrections, ensemble methods, shallow water extensions; other sensitivity analyses related to alternative spectral shape parameterizations

synthetic dataset(s)
updated version of NOMAD, hyperspectral version of NOMAD

implementation of algorithms & their modules in support of all science team members; provide a controlled environment for inter-comparisons & evaluations

discussion

comments regarding algorithms

comments regarding:

- data sets
- instrument needs / requirements
- uncertainties
- measurement methods / protocols
- use of additional environmental information

ZP Lee slides

Exact solution: $$r_{rs}(\lambda,\Omega') = L_u(0^-,\Omega') \Big/ E_d(0^-)$$ (Zaneveld 1995)

$$r_{rs}(\lambda,\Omega') \equiv \frac{D_d(\lambda,\theta_S')}{c(\lambda)+k_L(\lambda,\Omega')-f_L(\lambda,\Omega')b_f(\lambda)} \frac{\int_0^{2\pi}\int_0^{\pi/2}\beta(\Omega',\Omega)\,L(\lambda,\Omega')\sin(\theta')\,d\theta'\,d\varphi'}{E_{od}(0^-,\lambda,\theta_S')}$$

Gordon et al (1988)

$$r_{rs}(\lambda,0) = \sum_{i=1}^{2} g_i \left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^i$$

Albert and Mobley (2003) :

$$r_{rs}(\lambda,\Omega') = q(\Omega',w)\sum_{i=1}^{4} p_i \left(\frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^i$$

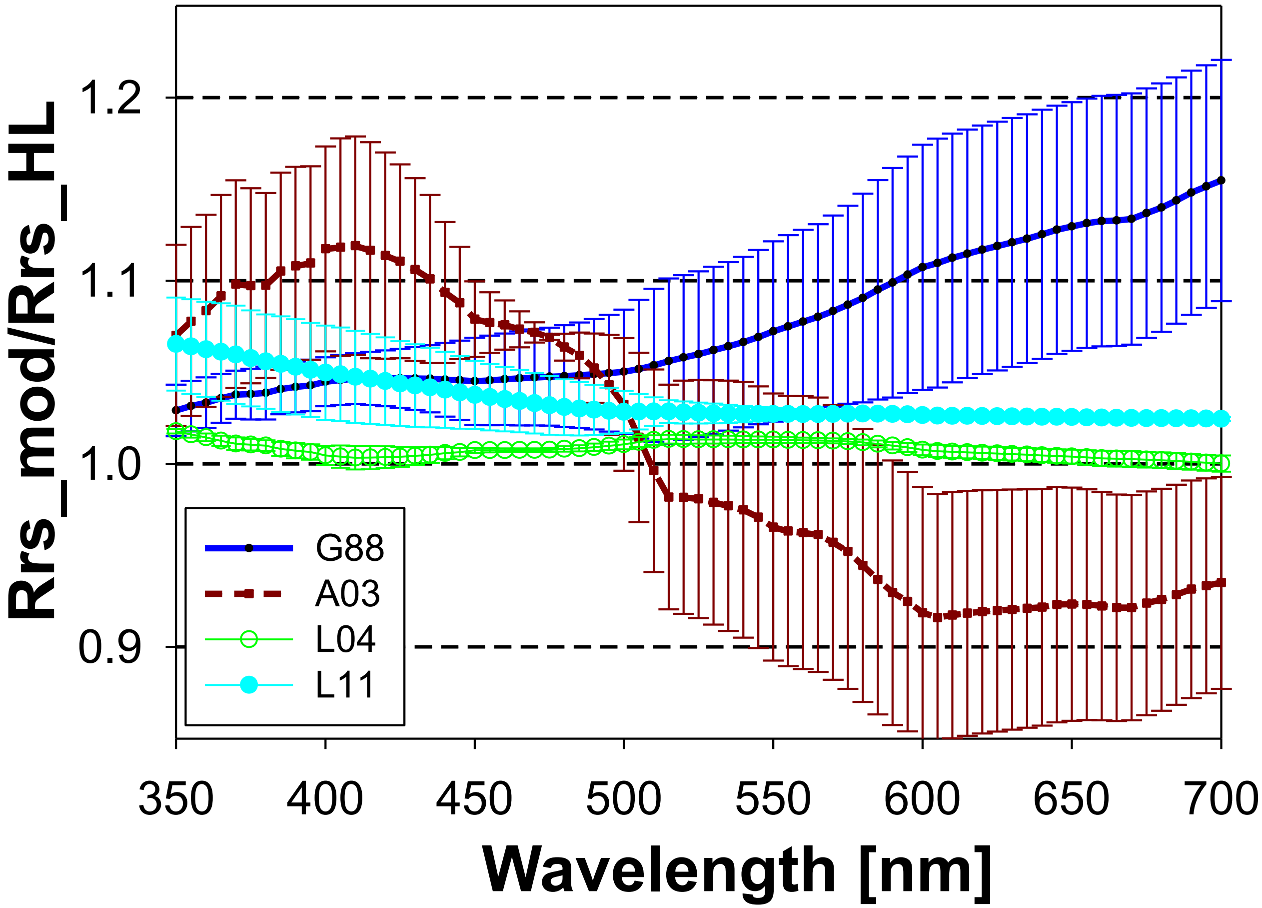
Lee et al (2004)

$$r_{rs}(\lambda,\Omega') = g_w(\Omega')\frac{b_{bw}(\lambda)}{a(\lambda)+b_b(\lambda)} + g_p(\lambda,\Omega')\frac{b_{bp}(\lambda)}{a(\lambda)+b_b(\lambda)}$$

$$g_p(\lambda,\Omega') = g_0\left(1-g_1 Exp\left(-g_2\frac{b_{bp}(\lambda)}{a(\lambda)+b_b(\lambda)}\right)\right)$$

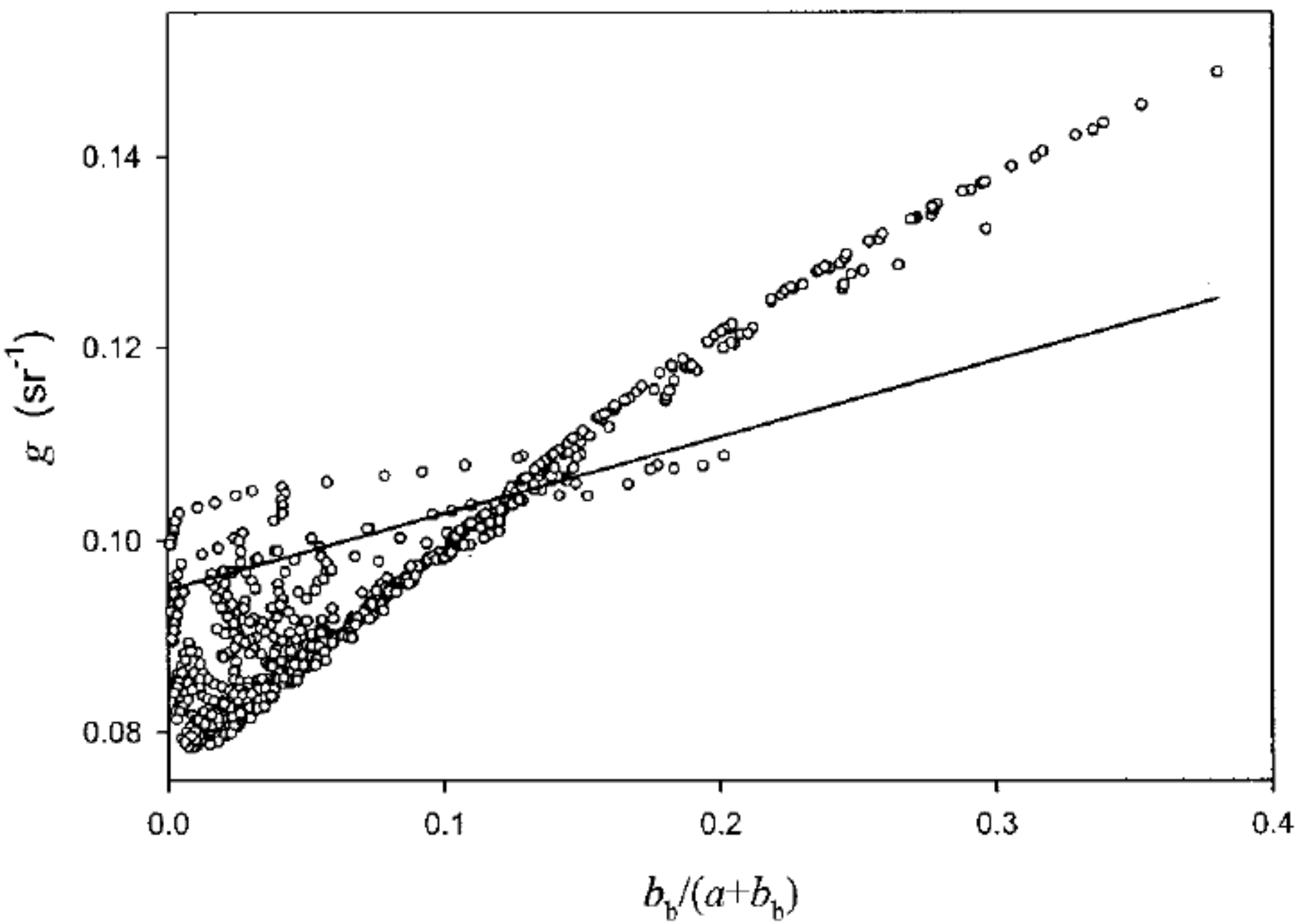
Lee et al (2011)

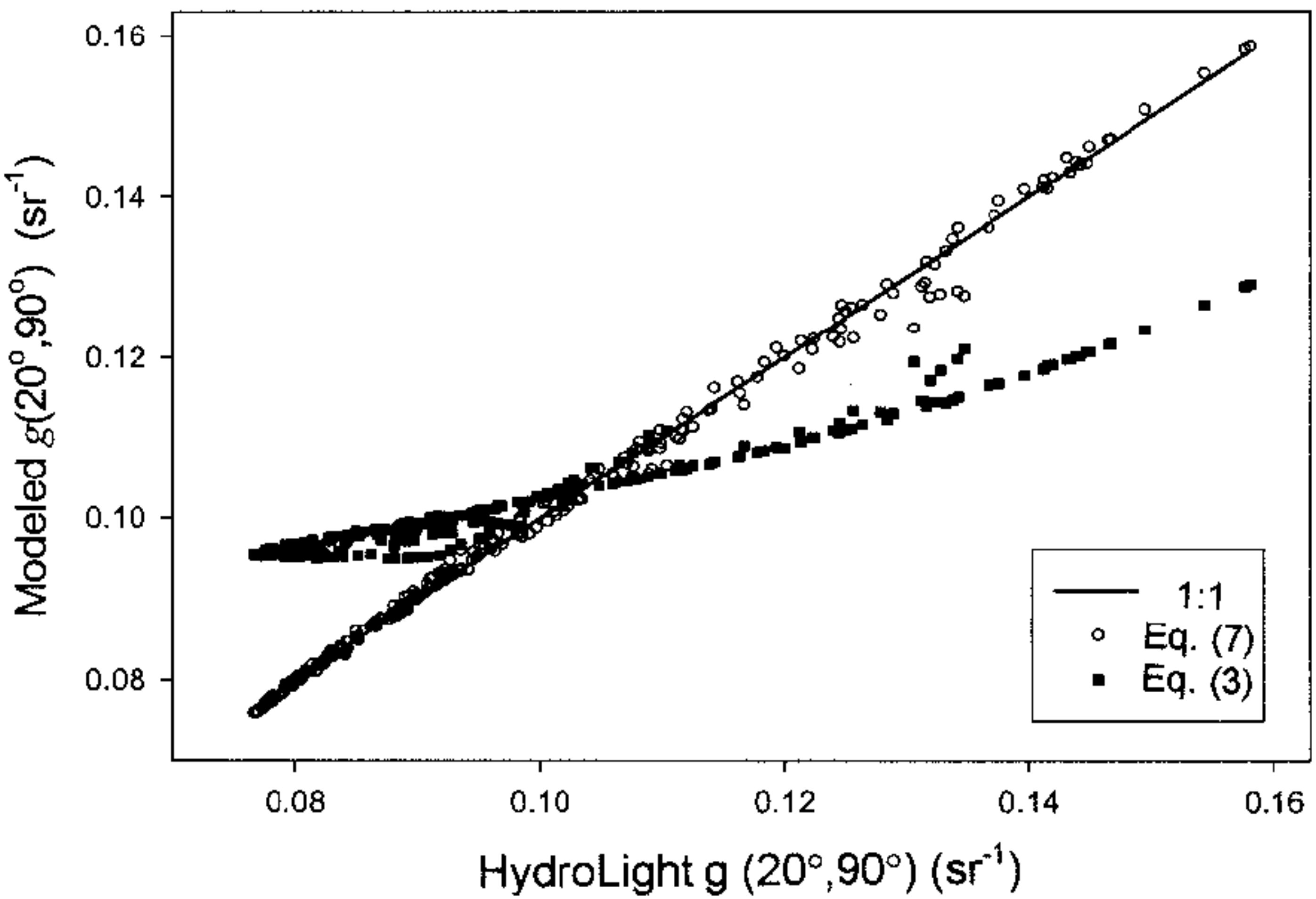
$$r_{rs}(\lambda,\Omega') = \sum_{i=1}^{2} g_i^w(\Omega')\left(\frac{b_{bw}(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^i + \sum_{i=1}^{2} g_i^p(\lambda,\Omega')\left(\frac{b_{bp}(\lambda)}{a(\lambda)+b_b(\lambda)}\right)^i$$



Rrs_mod/Rrs_HL
1.2
1.1
1.0
0.9
350
400
450
500
550
600
650
700
Wavelength [nm]
G88
A03
L04
L11

$$r_{rs}(\lambda) = g \frac{b_b(\lambda)}{a(\lambda) + b_b(\lambda)}$$



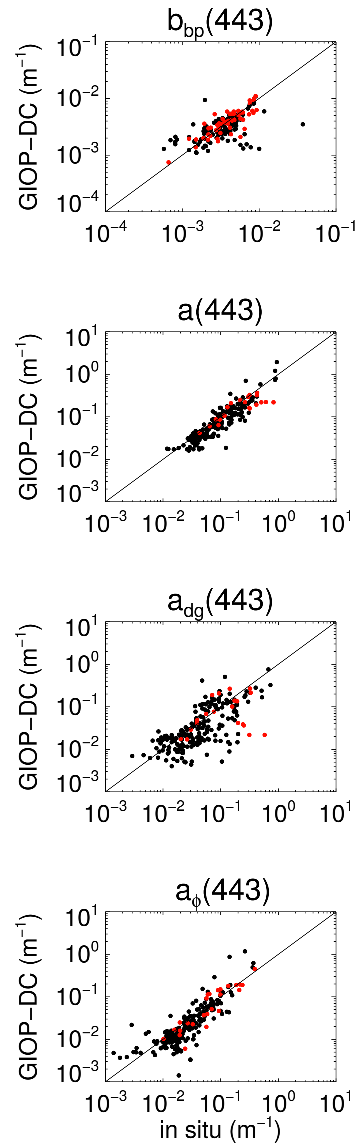


0.16
0.14
0.12
0.10
0.08
Modeled g(20°,90°) (sr⁻¹)
0.08
0.10
0.12
0.14
0.16
HydroLight g (20°,90°) (sr⁻¹)
1:1
Eq. (7)
Eq. (3)

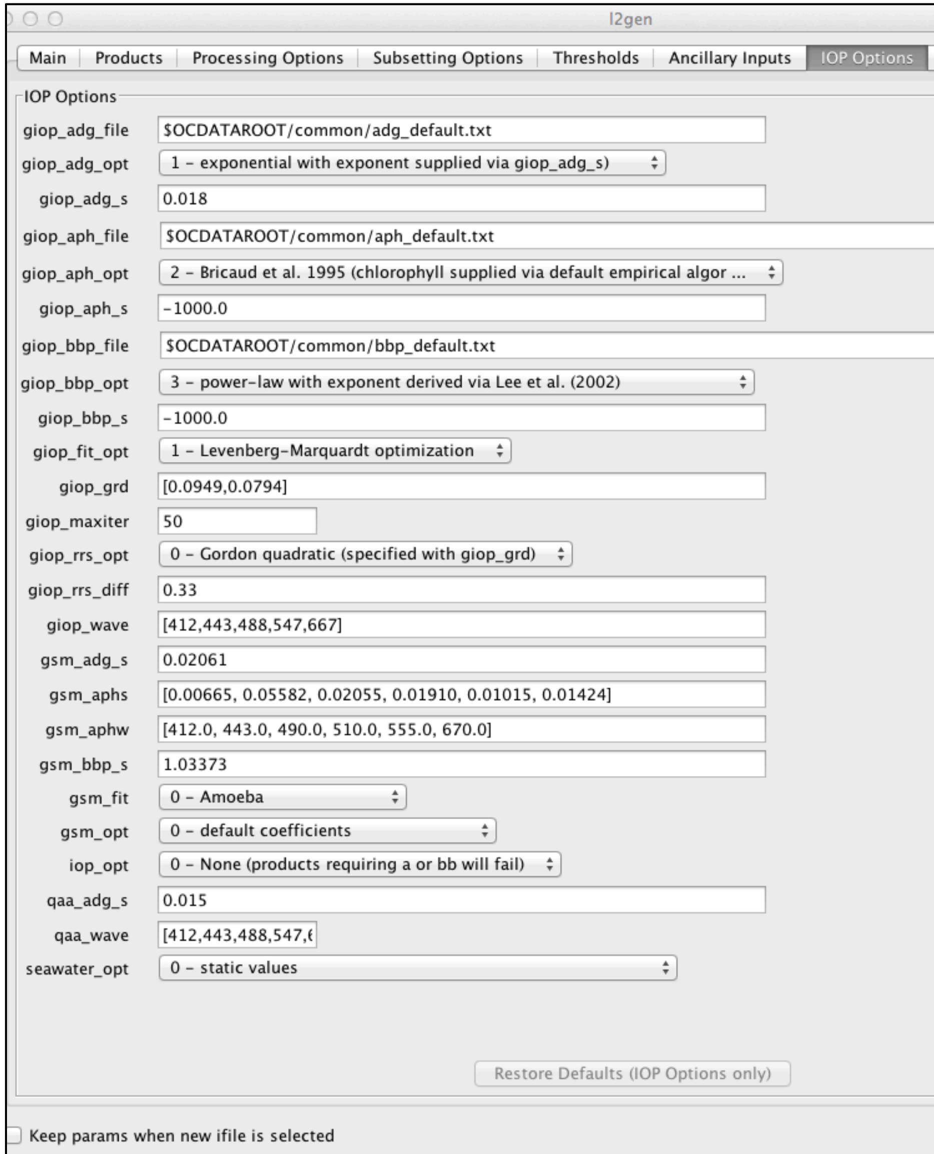
backup slides

satellite IOP match-ups

SeaWiFS & MODISA

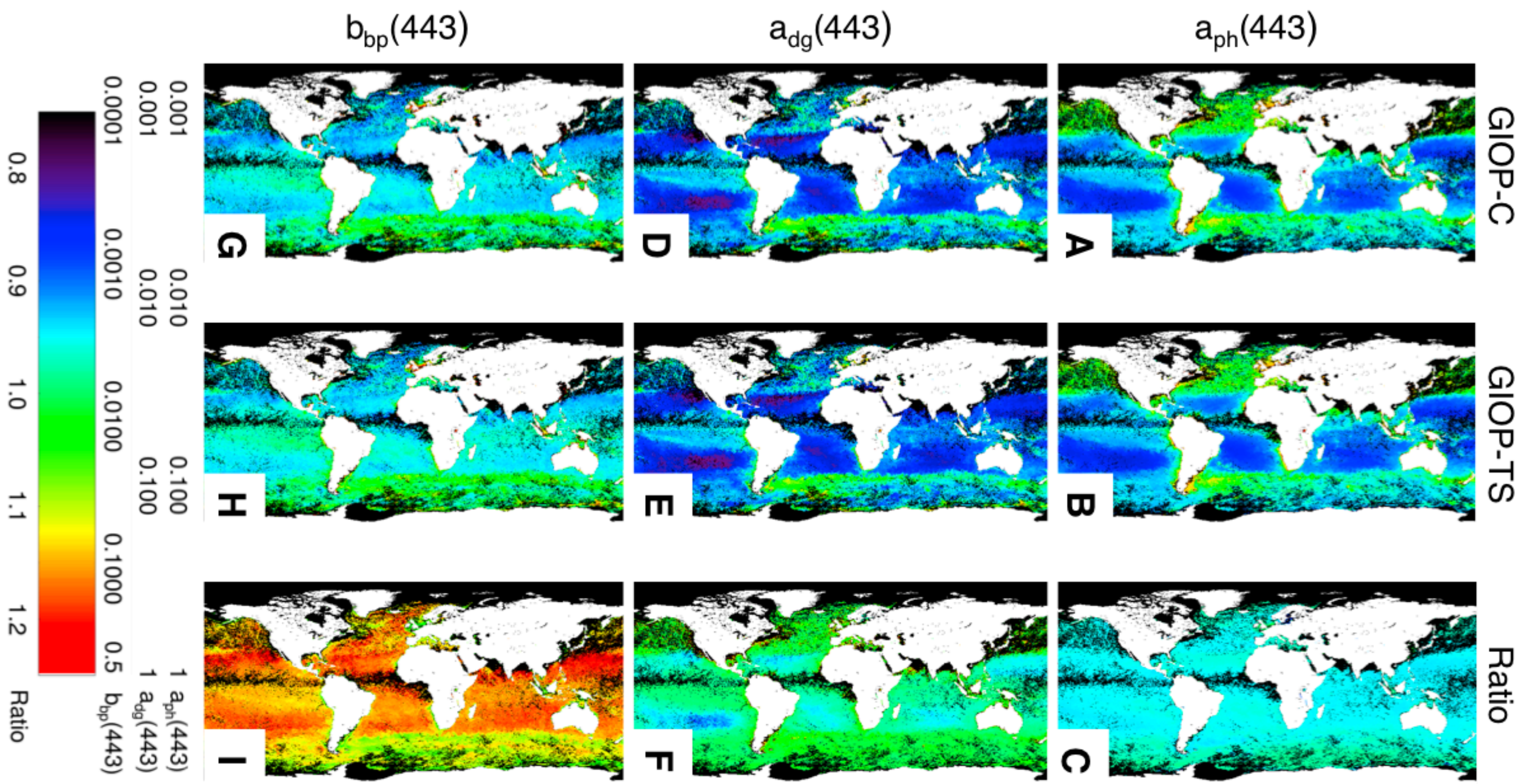


GIOP framework for PACE algorithm / module testing

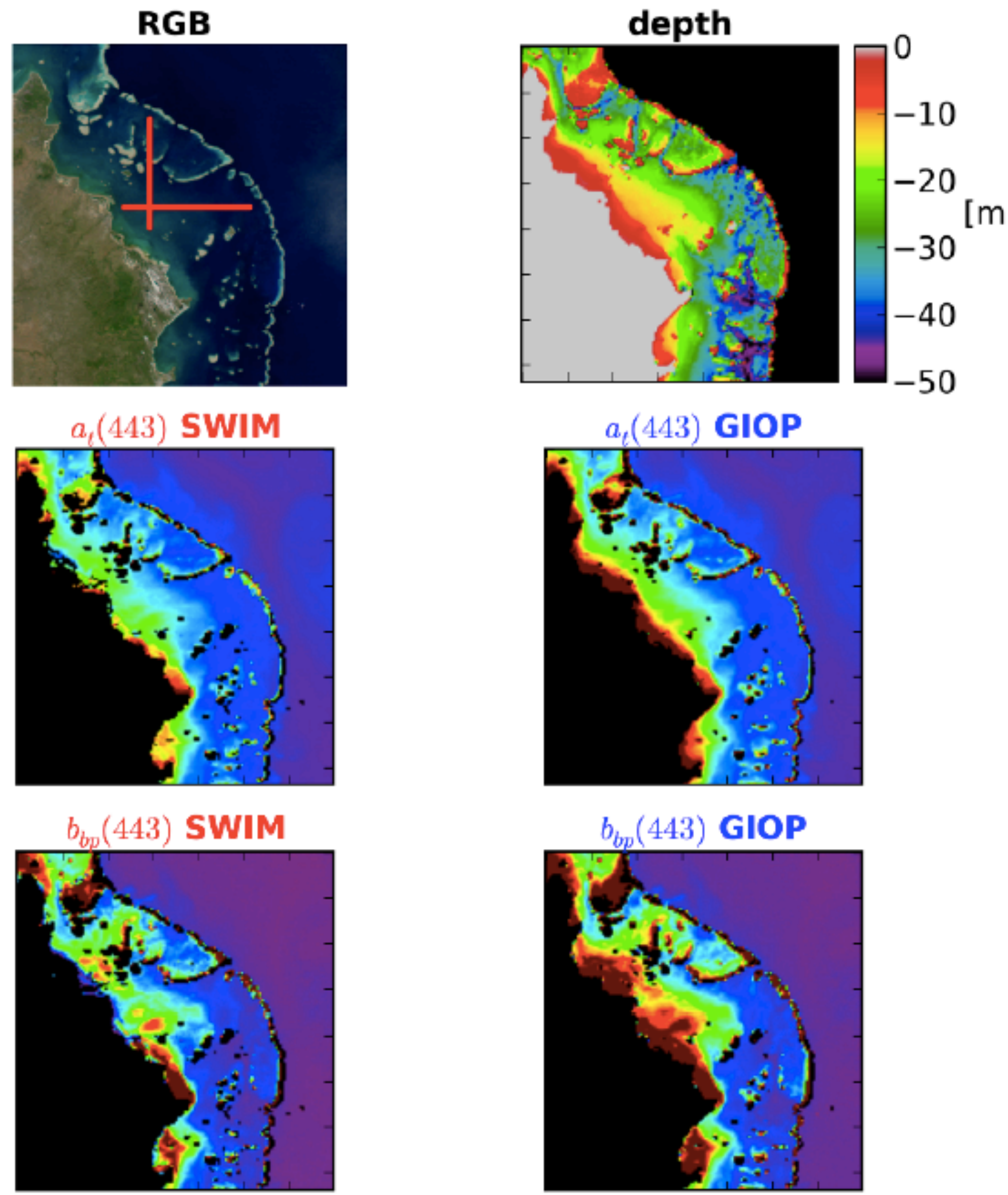


generalized IOP (GIOP) framework available through SeaDAS

temperature & salinity dependence of b_{bw}



optically shallow water



optically shallow water where sunlight reflected off the seafloor is seen by the satellite

SWIM and GIOP are similar algorithms, with the exception that SWIM has been extended to account for shallow water reflectances

Great Barrier Reef
McKinna et al. (2015)

configuring an IOP inversion algorithm

SAAs developed routinely over 30 yrs
many successfully retrieve **three** components
many overlapping approaches exist
GIOP defaults in red

power-law, η:
fixed
Lee et al. (2002)
Ciotti et al. (1999)
Hoge & Lyon (1996)
Loisel & Stramski (2001)
Morel (2001)

$$R_{rs} = G\left(\frac{b_{bw} + M_{bp} b^*_{bp}}{a_w + M_{dg} a^*_{dg} + M_{\phi} a^*_{\phi}}\right)$$

Levenberg-Marquardt
SVD matrix inversion

Morel f/Q
Gordon quadratic

exponential, S_{dg}:
fixed (= 0.018)
Lee et al. (2002)
Werdell (2010)
tabulated a^*_{dg}(l)

tabulated $a^*_{ph}(\lambda)$
Bricaud et al. (1998)
Ciotti & Bricaud (2006)